

```
ring/chain nodes:
24

chain bonds:
11-18 15-24

ring bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15 14-17 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 11-18 12-13 13-14 13-15 14-17 15-16 15-24 16-17 18-19 18-23 19-20 20-21 21-22 22-23
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Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS

=> d his

L1

(FILE 'HOME' ENTERED AT 17:19:11 ON 28 JUL 2004)

FILE 'REGISTRY' ENTERED AT 17:19:18 ON 28 JUL 2004

STRUCTURE UPLOADED

L2 QUE L1

L3 0 S L2

L4 83 S L2 SSS FUL

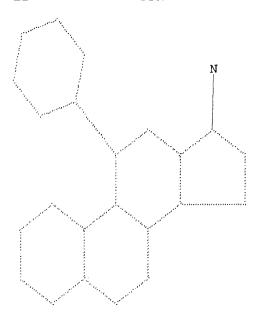
FILE 'CAPLUS' ENTERED AT 17:20:23 ON 28 JUL 2004

L5 3 S L4

=> d 12

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation. L2 QUE ABB=ON PLU=ON L1

=> d ibib abs hitstr 1-3

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10/61,1,785
    ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         2002:560363 CAPLUS
DOCUMENT NUMBER:
                         138:147491
TITLE:
                         Identification and characterization of novel estrogen
                         receptor-\beta-sparing antiprogestins
AUTHOR(S):
                         Sathya, Ganesan; Jansen, Michelle S.; Nagel, Susan C.;
                         Cook, C. Edgar; McDonnell, Donald P.
CORPORATE SOURCE:
                         Department of Pharmacology and Cancer Biology, Duke
                         University Medical Center, Durham, NC, 27710, USA
SOURCE:
                         Endocrinology (2002), 143(8), 3071-3082
                         CODEN: ENDOAO; ISSN: 0013-7227
PUBLISHER:
                         Endocrine Society
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
    The steroid hormones estrogen and progesterone together regulate the
    development and maintenance of the female reproductive system.
    actions of these two hormones are mediated by their resp. nuclear
    receptors located within overlapping cell populations in target organs.
    The mol. mechanism of action of these two hormones has been defined to a
    large extent using estrogen receptor (ER) and progesterone receptor (PR)
    antagonists. In the case of ER, the available antagonists are highly
    receptor selective. With respect to PR, however, the available
    antiprogestins also interact with the receptors for glucocorticoids,
    mineralocorticoids, and androgens. Whereas these cross-reactivities can
    usually be managed in studies of female reproductive function, it is the
    recent demonstration that RU486 is an effective antagonist of the
    \beta-isoform of ER that suggested the need for more selective
    antiprogestins. In this study, we used cell-based transcriptional assays
    combined with screens using coactivator peptide analogs to identify two
    novel classes of antiprogestins that distinguish themselves from the
    antiprogestin RU486 in the manner they interact with PR. One class
    exhibits the characteristics of a pure antiprogestin in that its members
    bind to the receptor and induce a conformational change that prevents the
    presentation of two potential coactivator binding surfaces on the protein.
    The second class of compds. distinguish themselves from RU486 in that they
    are ER\beta sparing. When tested in vivo the ER-sparing antiprogestins
    were as effective as RU486 in suppressing superovulation. It is
    anticipated that the availability of these new antiprogestins will advance
    the studies of PR pharmacol. in a manner similar to how the availability
    of selective ER modulators has helped the study of ER action.
    244304-81-2, RTI 6413-015 244304-82-3, RTI 6413-045
    244304-85-6, RTI 6413-029E 244304-86-7, RTI 6413-045ox
    244304-89-0, RTI 6413-013 244304-91-4, RTI 6413-028
    244305-03-1, RTI 6413-044 244305-17-7, RTI 6413-029Z
    496840-89-2, RTI 6413-030 496840-92-7, RTI 6413-043
    496840-93-8, RTI 6413-043ox
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
    (Biological study); USES (Uses)
        (identification and characterization of novel estrogen
```

Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-17-

Absolute stereochemistry.

244304-81-2 CAPLUS

receptor- β -sparing antiprogestins)

nitro-, $(11\beta, 17\beta)$ - (9CI) (CA INDEX NAME)

RN

CN

RN 244304-82-3 CAPLUS

CN Estra-4,9-dien-3-one, 17-(3-hydroxypropyl)-11-[4-(methylthio)phenyl]-17-nitro-, $(11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244304-85-6 CAPLUS

CN Estra-4,9-dien-3-one, $11-(4-acetylphenyl)-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 244304-86-7 CAPLUS

CN Estra-4,9-dien-3-one, 17-(3-hydroxypropyl)-11-[4-(methylsulfinyl)phenyl]-

Page 3

17-nitro-,
$$(11\beta, 17\beta)$$
- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244304-89-0 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-nitro-17-(1-propynyl)-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244304-91-4 CAPLUS

CN Estra-4,9-dien-3-one, 11-(4-acetylphenyl)-17-nitro-17-(1-propynyl)-, $(11\beta,17\beta)-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-03-1 CAPLUS

CN Estra-4,9-dien-3-one, $17-(3-hydroxy-1-propenyl)-11-[4-(methylthio)phenyl]-17-nitro-, <math>(11\beta,17\beta)-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 244305-17-7 CAPLUS

CN Estra-4,9-dien-3-one, $11-(4-acetylphenyl)-17-[(1Z)-3-hydroxy-1-propenyl]-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 496840-89-2 CAPLUS

CN 19-Norpregna-4,9-dien-3-one, 11-(4-acetylphenyl)-21-hydroxy-17-nitro-, $(11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

10/611,785

RN 496840-92-7 CAPLUS

CN Estra-4,9-dien-3-one, 11-[4-(methylthio)phenyl]-17-nitro-17-(1-propynyl)-, $(11\beta,17\beta)-(9CI)$ (CA INDEX NAME)

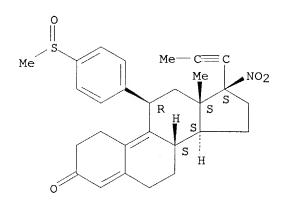
Absolute stereochemistry.

RN 496840-93-8 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(methylsulfinyl)phenyl]-17-nitro-17-(1-propynyl)-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Currently available stereo shown.



54

REFERENCE COUNT:

THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

X 10/611,785

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:784119 CAPLUS

DOCUMENT NUMBER:

132:23141

TITLE:

Preparation of 17β -amino- and

 17β -hydroxylamino- 11β -arylsteroids with

potent antiprogestational activity

INVENTOR(S):

Cook, C. Edgar; Kepler, John A.; Bartley, Gary S.;

Shetty, Rupa S.

PATENT ASSIGNEE(S):

Research Triangle Institute, USA

SOURCE:

PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	KIND DATE					APPLICATION NO. DATE													
WO	WO 9962928				A1 19991209				WO 1999-US10480							19990528			
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															IS,				
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		NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE	, S	G,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	
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	R 9910794																		
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			FI,																
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NZ	NZ 507985			A		2003		NZ 1999-507985						1999	0528				
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										_					1999				
										200	1-8	9539	95	Al	2001	0702			
THER S	OURCE	(S):		MARPAT 132:23141															

GΙ

 11β -Phenylestradienes I [R1 = R2R3N(O)m, nitrogen containing AΒ heterocyclyl; R2, R3 = H, alkyl, cycloalkyl alkenyl; R6 = H, alkyl, halogen; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R8, R9 = H, OH, alkyl, alkenyl, alkynyl, acyl, alkyloxy; R13 = H, halogen; R1R12 = fused nitrogen containing heterocyclic ring; X = H2, OH, silyloxy, acyloxy, etc.; m, n = 0, 1] and II [R1 = R2R3N(O)m, nitrogen containing heterocyclyl; R2, R3 = H, alkyl, cycloalkyl alkenyl; R6 = H, alkyl, halogen; R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R9 = H, OH, alkyl, alkenyl, alkynyl, acyl, alkyloxy; R13 = H, halogen; R1R12 = fused nitrogen containing heterocyclic ring; X = H2, OH, silyloxy, acyloxy, etc.; Y = CR13R14; Z = CH2, C:CH2; R13, R14 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R13R14 = 0; m, n = 0, 1] were prepared and exhibited potent antiprogestational activity. Thus, oxime III (R = 4-dimethylaminophenyl) was prepared starting from sterol IV (R = 4-dimethylaminophenyl) in two steps. The prepared compds. were tested for progesterone receptor binding activity, progestational activity, and antiprogestational activity.

IT 251987-44-7P 251987-54-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 17 β -amino- and 17 β -hydroxylamino-11 β - phenylestradienes with potent antiprogestational activity) 251987-44-7 CAPLUS

RN 251987-44-7 CAPLUS CN Estra-4,9-dien-3-one, 17-amino-11-[4-(dimethylamino)phenyl]-17-(1-propynyl)-, $(11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 251987-54-9 CAPLUS CN Estra-4,9-dien-3-one, 17-amino-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, (11β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

251987-35-6P 251987-40-3P 251987-48-1P

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251987-52-7P 251987-58-3P 251987-62-9P
     251987-65-2P 251988-38-2P 251988-39-3P
     251988-40-6P 251988-41-7P 251988-42-8P
     251988-43-9P 251988-45-1P 251988-46-2P
     251988-47-3P 251988-48-4P 251988-49-5P
     251988-50-8P 251988-52-0P 251988-53-1P
     251988-54-2P 251988-55-3P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of 17\beta-amino- and 17\beta-hydroxylamino-11\beta-
        phenylestradienes with potent antiprogestational activity)
RN
     251987-35-6 CAPLUS
     Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-(hydroxyamino)-17-(1-
CN
     propynyl) -, (11\beta, 17\beta) - (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

IT

RN 251987-40-3 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-(hydroxymethylamino)-17-(1-propynyl)-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251987-48-1 CAPLUS

CN Acetamide, N-[$(11\beta,17\beta)$ -11-[4-(dimethylamino)phenyl]-3-oxo-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} - \text{C} & \text{C} \\ \text{Me} & \text{NHAC} \\ \\ \text{R} & \text{S} \\ \\ \text{S} & \text{H} \\ \end{array}$$

RN 251987-52-7 CAPLUS

CN Estra-4,9-dien-3-one, 17-(dimethylamino)-11- $\{4-(dimethylamino)phenyl\}-17-(1-propynyl)-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

RN 251987-58-3 CAPLUS

CN Estra-4,9-dien-3-one, 17-(hydroxyamino)-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251987-62-9 CAPLUS

CN Formamide, N-[$(11\beta,17\beta)$ -17-[3-(formyloxy)propyl]-3-oxo-11-[4-(1-piperidinyl)phenyl]estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251987-65-2 CAPLUS

CN Formamide, $N-[(11\beta,17\beta)-17-(3-hydroxypropyl)-3-oxo-11-[4-(1-piperidinyl)phenyl]estra-4,9-dien-17-yl]-(9CI) (CA INDEX NAME)$

Absolute stereochemistry.

RN 251988-38-2 CAPLUS

CN Estra-4,9-dien-3-one, 17-(hydroxyamino)-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)-, $(11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-39-3 CAPLUS

CN Estra-4,9-dien-3-one, 17-(hydroxymethylamino)-11-[4-(1-piperidinyl)phenyl]- 17-(1-propynyl)-, $(11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 251988-40-6 CAPLUS

CN Estra-4,9-dien-3-one, 17-amino-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)-, $(11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-41-7 CAPLUS

CN Acetamide, N-[(11 β ,17 β)-3-oxo-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

RN 251988-42-8 CAPLUS

CN Formamide, N-[$(11\beta,17\beta)$ -11-[4-(dimethylamino)phenyl]-3-oxo-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-43-9 CAPLUS

CN Formamide, $N-[(11\beta,17\beta)-11-[4-(dimethylamino)phenyl]-3-oxo-17-(1-propynyl)estra-4,9-dien-17-yl]-N-hydroxy- (9CI) (CA INDEX NAME)$

Absolute stereochemistry.

RN 251988-45-1 CAPLUS

CN Formamide, N-[$(11\beta,17\beta)$ -3-oxo-11-[4-(1-piperidinyl)phenyl]-17-(1-propynyl)estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-46-2 CAPLUS

CN Formamide, N-hydroxy-N-[$(11\beta,17\beta)$ -3-oxo-11-[4- $(1-\beta)$ -4- $(1-\beta)$ -4- $(1-\beta)$ -4- $(1-\beta)$ -5-0xo-11-[4- $(1-\beta)$ -6- $(1-\beta)$ -7- $(1-\beta)$ -7- $(1-\beta)$ -8-0xo-11-[4- $(1-\beta)$ -8-1- $(1-\beta)$ -8-

Absolute stereochemistry.

RN 251988-47-3 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-(hydroxyamino)-17-(3-hydroxypropyl)-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

RN 251988-48-4 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-(hydroxymethylamino)-17-(3-hydroxypropyl)-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-49-5 CAPLUS

CN Estra-4,9-dien-3-one, 17-(hydroxymethylamino)-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, (11 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-50-8 CAPLUS

CN Estra-4,9-dien-3-one, 17-amino-11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-, $(11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-52-0 CAPLUS

CN Acetamide, N-[$(11\beta,17\beta)$ -11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-3-oxoestra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-53-1 CAPLUS

CN Acetamide, N-[$(11\beta,17\beta)$ -17-(3-hydroxypropyl)-3-oxo-11-[4-(1-piperidinyl)phenyl]estra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-54-2 CAPLUS

CN Formamide, N-[$(11\beta, 17\beta)$ -11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-3-oxoestra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-55-3 CAPLUS CN Formamide, N-[$(11\beta,17\beta)$ -11-[4-(dimethylamino)phenyl]-17-[3-(formyloxy)propyl]-3-oxoestra-4,9-dien-17-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 244305-29-1 251988-37-1

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of 17β -amino- and 17β -hydroxylamino- 11β -phenylestradienes with potent antiprogestational activity)

RN 244305-29-1 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 251988-37-1 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, ethyl ester, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251987-83-4 CAPLUS

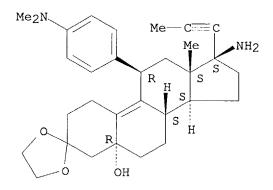
CN Estr-9-en-3-one, $11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(hydroxymethylamino)-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, <math>(5\alpha,11\beta,17\beta)-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 251987-87-8 CAPLUS

CN Estr-9-en-3-one, 17-amino-11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 251988-11-1 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-14-4 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-17-7 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, methyl ester, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

RN 251988-20-2 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251988-22-4 CAPLUS

CN Estr-9-en-3-one, 17-amino-5-hydroxy-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 251988-24-6 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(hydroxyamino)-17-(3-hydroxypropyl)-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, (5α,11β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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10/611,785
     ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
                         1999:633297 CAPLUS
ACCESSION NUMBER:
                          131:243468
DOCUMENT NUMBER:
                          Preparation of 17\beta-nitro-11\beta-arylsteroids
TITLE:
                          and their derivatives having agonist or antagonist
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hormonal properties

INVENTOR(S): Cook, C. Edgar; Kepler, John A.; Shetty, Rupa S.; Bartley, Gary S.; Lee, David Yue-Wei

Research Triangle Institute, USA

PATENT ASSIGNEE(S): SOURCE:

U.S., 24 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.					D DATE			APPLICATION NO.						DATE			
	5 5962444			A 199910				US 1998-86674					19980529					
US	US 6015805			Α		2000		τ	JS 19	99-3	5	19990525						
		2333668																
WO	9962929			A1					WO 1999-US10481 19990528									
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		KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	
		NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	
		UA,	UG,	UZ,	VN,	YU,	ZW,	AM,	AΖ	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM		
	RW:	GH,	GM,	ΚE,	LS,	MW,	SD,	SL,	SZ	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,	
		ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	
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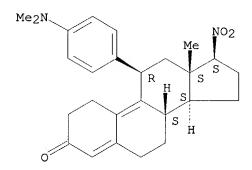
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$$R^2$$
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AΒ 17β -Nitro- 11β -arylsteroids of formula I [R1 = (substituted) amino, halo, OH, alkoxy, alkylthio, acyl, etc.; R2 = H, halo; R3 = H, alkyl, alkenyl, alkynyl, aryl, etc.; R4 = H, alkyl, halo; X = O, (substituted) NOH] are prepared The compds. exhibit potent antiprogestational activity and are useful in the treatment of fibroids, endometriosis, cervical ripening prior to delivery, hormone replacement therapy and in the control of fertility. Thus, 3,3-(1,2-ethanedioxy)estra-5(10), 9(11) -dien-17-one was transformed into II in several steps. The affinity of II for human progesterone hormone receptor was IC50 of 0.8 nM. 244304-80-1P 244304-81-2P 244304-82-3P 244304-83-4P 244304-84-5P 244304-85-6P 244304-86-7P 244304-89-0P 244304-90-3P 244304-91-4P 244305-03-1P 244305-17-7P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 17β -nitro- 11β -arylsteroids and derivs. with progestational or antiprogestational activity) RN 244304-80-1 CAPLUS CN Estra-4,9-dien-3-one, 11-[4-(dimethylamino)phenyl]-17-nitro-, $(11\beta, 17\beta)$ - (9CI) (CA INDEX NAME)

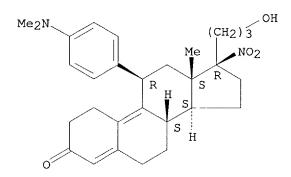
Absolute stereochemistry.



RN 244304-81-2 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-(3-hydroxypropyl)-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 244304-82-3 CAPLUS

CN Estra-4,9-dien-3-one, $17-(3-hydroxypropyl)-11-[4-(methylthio)phenyl]-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244304-83-4 CAPLUS

CN Estra-4,9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 244304-84-5 CAPLUS

CN Estra-4,9-dien-3-one, $11-(4-acetylphenyl)-17-(3-hydroxypropyl)-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

RN 244304-85-6 CAPLUS

CN Estra-4,9-dien-3-one, $11-(4-acetylphenyl)-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 244304-86-7 CAPLUS

CN Estra-4,9-dien-3-one, 17-(3-hydroxypropyl)-11-[4-(methylsulfinyl)phenyl]-17-nitro-, (11β,17β)- (9CI) (CA INDEX NAME)

RN 244304-89-0 CAPLUS

CN Estra-4, 9-dien-3-one, $11-[4-(dimethylamino)phenyl]-17-nitro-17-(1-propynyl)-, (11<math>\beta$, 17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me-C} = \text{C} \\ \text{Me} \\ \text{S} \\ \text{S} \\ \text{H} \\ \\ \text{O} \\ \end{array}$$

RN 244304-90-3 CAPLUS

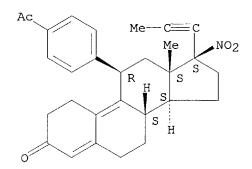
CN 19-Norpregna-4,9-dien-20-yn-3-one, 11-(4-acetylphenyl)-17-nitro-, $(11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244304-91-4 CAPLUS

CN Estra-4,9-dien-3-one, 11-(4-acetylphenyl)-17-nitro-17-(1-propynyl)-, $(11\beta,17\beta)-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 244305-03-1 CAPLUS

CN Estra-4,9-dien-3-one, 17-(3-hydroxy-1-propenyl)-11-[4-(methylthio)phenyl]-17-nitro-, (11β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 244305-17-7 CAPLUS

CN Estra-4,9-dien-3-one, $11-(4-acetylphenyl)-17-[(1Z)-3-hydroxy-1-propenyl]-17-nitro-, (11<math>\beta$,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 244305-38-2

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of 17β -nitro- 11β -arylsteroids and derivs. with progestational or antiprogestational activity)

RN 244305-38-2 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 1,2-ethanediyl acetal, (5α ,11 β)- (9CI) (CA INDEX NAME)

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IT
     244304-96-9P 244304-97-0P 244304-98-1P
     244304-99-2P 244305-00-8P 244305-01-9P
     244305-02-0P 244305-04-2P 244305-06-4P
     244305-07-5P 244305-09-7P 244305-10-0P
     244305-11-1P 244305-12-2P 244305-13-3P
     244305-14-4P 244305-15-5P 244305-16-6P
     244305-19-9P 244305-20-2P 244305-21-3P
     244305-22-4P 244305-23-5P 244305-24-6P
     244305-26-8P 244305-29-1P 244305-32-6P
     244305-33-7P 244305-34-8P 244305-36-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of 17\beta-nitro-11\beta-arylsteroids and derivs. with
        progestational or antiprogestational activity)
     244304-96-9 CAPLUS
RN
     Estr-9-en-3-one, 17-bromo-11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-
CN
     , cyclic 1,2-ethanediyl acetal, (5\alpha,11\beta)- (9CI) (CA INDEX
    NAME)
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Absolute stereochemistry.

RN 244304-97-0 CAPLUS CN Estr-9-en-3-one, $11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 1,2-ethanediyl acetal, <math>(5\alpha,11\beta,17\beta)-(9CI)$ (CA INDEX NAME)

10/611,785

Absolute stereochemistry.

RN 244304-98-1 CAPLUS

CN Estr-9-en-3-one, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244304-99-2 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 11-[3-bromo-4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

RN 244305-00-8 CAPLUS

CN Estr-9-en-3-one, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-(3-hydroxypropyl)-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-01-9 CAPLUS CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-(3-

hydroxypropyl)-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 244305-02-0 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 11-[4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-04-2 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 11-[3-bromo-4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, (5α,11β,17α,20Ε)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 244305-06-4 CAPLUS

CN Estr-9-en-3-one, 11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 244305-07-5 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-[(1E)-3-hydroxy-1-propenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 244305-09-7 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta)$ -(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-10-0 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta)$ - (9CI) (CA INDEX NAME)

RN 244305-11-1 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, methyl ester, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-12-2 CAPLUS

CN 19-Norpregn-9-ene-21-carboxaldehyde, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

RN 244305-13-3 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-14-4 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, methyl ester, $(5\alpha,11\beta,17\alpha,20E)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 244305-15-5 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, methyl ester, $(5\alpha,11\beta,17\alpha,20Z)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 244305-16-6 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-[(1E)-3-hydroxy-1-propenyl]-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 244305-19-9 CAPLUS

CN Estr-9-en-3-one, 17-bromo-5-hydroxy-11-[4-(methylsulfinyl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-20-2 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(methylsulfinyl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta)$ - (9CI) (CA INDEX NAME)

RN 244305-21-3 CAPLUS

CN 19-Norpregn-9-ene-21-carboxylic acid, 3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-11-[4-(methylsulfinyl)phenyl]-17-nitro-, methyl ester, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-22-4 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-11-[4-(methylthio)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 244305-23-5 CAPLUS CN Estr-9-en-3-one, 5-hydroxy-17-(3-hydroxypropyl)-11-[4-

(methylsulfinyl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-24-6 CAPLUS

CN 19,21-Dinorchol-9-ene-3,23-dione, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 3-(1,2-ethanediyl acetal), (5α,11β,17α)- (9CI) (CA INDEX NAME)

RN 244305-26-8 CAPLUS

CN 19,21-Dinorchol-9-ene-3,23-dione, $11-[3-bromo-4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-, cyclic 3-(1,2-ethanediyl acetal), (5<math>\alpha$,11 β ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-29-1 CAPLUS

CN Estr-9-en-3-one, 11-[4-(dimethylamino)phenyl]-5-hydroxy-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 244305-32-6 CAPLUS

CN 19-Norpregn-9-en-20-yn-3-one, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-33-7 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(2-methyl-1,3-dioxolan-2-yl)phenyl]-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 244305-34-8 CAPLUS

CN 19-Norpregn-9-ene-21-carboxaldehyde, $11-[4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, <math>(5\alpha,11\beta,17\alpha)-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 244305-36-0 CAPLUS

CN 19,21-Dinorchol-9-ene-3,23-dione, 5-hydroxy-17-nitro-11-[4-(1-piperidinyl)phenyl]-, cyclic 3-(1,2-ethanediyl acetal), $(5\alpha,11\beta,17\alpha)$ - (9CI) (CA INDEX NAME)

IT 244305-05-3P 244305-30-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 17β -nitro- 11β -arylsteroids and derivs. with progestational or antiprogestational activity)

RN 244305-05-3 CAPLUS

CN 19-Norpregna-9,20-diene-21-carboxylic acid, $11-[3-bromo-4-(dimethylamino)phenyl]-3,3-[1,2-ethanediylbis(oxy)]-5-hydroxy-17-nitro-, methyl ester, <math>(5\alpha,11\beta,17\alpha,202)-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 244305-30-4 CAPLUS

CN Estr-9-en-3-one, 5-hydroxy-11-[4-(methylamino)phenyl]-17-nitro-17-(1-propynyl)-, cyclic 1,2-ethanediyl acetal, $(5\alpha,11\beta,17\beta)$ - (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT